Glutaric acid, 3-methylbut-2-en-1-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C17H30O5/c1-14(2)8-12-21-16(18)6-5-7-17(19)22-13-10-15(3)9-11-20-4/h8,15

InchiKey: HVHQQXIBVIMXJJ-UHFFFAOYSA-N

Formula: C17H30O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-411.35	kJ/mol	Joback Method
hf	-913.88	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.272		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	766.96	K	Joback Method
tc	952.45	K	Joback Method
tf	413.86	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.35	J/mol×K	766.96	Joback Method
cpg	813.87	J/mol×K	797.87	Joback Method
cpg	829.47	J/mol×K	828.79	Joback Method
cpg	844.15	J/mol×K	859.70	Joback Method
cpg	857.93	J/mol×K	890.62	Joback Method
cpg	870.82	J/mol×K	921.53	Joback Method
cpg	882.83	J/mol×K	952.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393520&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume